JOURNAL OF MOLECULAR STRUCTURE, VOLUME 161 (1987)

AUTHOR INDEX

Ács, M. 111
Aehle, W. 63
Ardid, I. 151
Argay, Gy. 125
Arias, M. S. 151
Avci, G. F. 205

Balogh, G. 111
Bates, P. A. 181
Beagley, B. 105
Bellanato, J. 151
Bernáth, G. 125
Berthault, P. 175
Bodot, H. 265
Bonnet, J.-P. 175
Boros, I. 111
Bulanin, M. O. 321
Bulychev, V. P. 321

Charbonnier, S. 265
Colomban, Ph. 1

De Meijere, A. 97
Dryanska, V. 231
Duddeck, H. 231
Duncan, J. L. 311

Edwards, H. G. M. 23
Emsley, J. 181, 193

Faigl, F. 111
Faria, D. L. A. 15
Fleck, S. 139
Florencio, F. 151
Fogassy, E. 111
Ford, T. A. 245
Foulds, G. A. 237
Freeman, N. J. 181, 193
Fülöp, F. 125

Galvez, E. 151
Garcia-Blanco, S. 151
Garcia-Ramos, J. V. 151
Gardiner, D. J. 55
Göckel, R. 139
Guohai, L. 75
Guozhen, W. 75

Hall, P. S. 237
Harmon, K. M. 205
Hidasi, G. 111
Horn, A. 63
Hursthouse, M. B. 181

Ivanov, C. 231

Kaiser, M. 231
Kálmán, A. 125
Kasende, O. 87
Kim, K. 297
Klaeboe, P. 63
Knowles, R. K. 105

Labarre, J.-F. 175
Lis, T. 165

Majerz, I. 165
Malarski, Z. 165
Merz, H. 87
Mikhova, B. 231
Munro, B. 311

Nielsen, C. J. 63
Novak, A. 1

Owen, N. L. 33

Palmer, M. H. 333
Park, C. W. 297
Perly, B. 175
Pham-Thi, M. 1
Popandova, K. 231
Pourcin, J. 265
Prasad, N. V. L. N. 219
Premaswarup, D. 219
Pritchard, R. G. 105

Rastogi, P. P. 87

Santos, J. G. N. 15
Santos, P. S. 15
Schmideder, H. 87
Simon, K. 111
Smith, C. H. 33
Spassov, S. L. 231
Stavnebrekk, P. J. 283
Stølevik, R. 283

Thiel, A. C. 205
Thornton, D. A. 237
Tokhadze, K. G. 321
Traetteberg, M. 97

Venkatacharyulu, P. 219
Viani, R. 265
Vidaud, L. 175

Walker, N. A. 55
Weaving, J. S. 245
Weiss, A. 139
Williams, G. A. 33

Zundel, G. 87

JOURNAL OF MOLECULAR STRUCTURE, VOLUME 161 (1987)

SUBJECT INDEX

Barrelene,
a re-interpretation of the uv-photoelectron spectra of Dewar benzene, norbornadiene and barrelene by ab initio configuration interaction calculations 333
Benzidine,
surface enhanced Raman study of benzidine on a silver electrode: an interpretation for different adsorption configurations at various applied voltages 75
Benzothiazines,
on the tautomerism and conformational characteristics of 2-phenylimino-3,1-perhydrobenzoxazines and analogous benzothiazines: an X-ray study 125
Bromocyclohexane,
conformational enthalpy and volume changes in bromocyclohexane determined by Raman spectroscopy 55

Caesium hydrogen selenate ($CsHSeO_4$),
vibrational study of structures and phase transitions in caesium hydrogen selenate ($CsHSeO_4$) 1

Dewar benzene,
a re-interpretation of the uv-photoelectron spectra of Dewar benzene, norbornadiene and barrelene by ab initio configuration interaction calculations 333
Diacetylene,
vibrational spectra of diacetylene and its deuterated species 33
2,6-Dichlorophenol
single crystal Zeeman effect studies on ^{35}Cl NQR lines of 2,6-dichlorophenol 219
β-Diketone interactions,
β-diketone interactions. Part 4. The structures and properties of 1,3-diphenyl-2-methylpropane-1,3-dione, $C_{16}H_{14}O_2$, and 1,3-diphenyl-2-(4-methoxyphenyl) propane-1,3-dione, $C_{22}H_{18}O_3$ 181
β-Diketone interactions,
β-diketone interactions. Part 5. Solvent effects on the keto ⇌ enol equilibrium 193
1,1′-Dimethyl-bicyclopropyl,
the molecular structure and conformation of 1,1′-dimethylbicyclopropyl 97
1,3-Diphenyl-2-(4-methoxyphenyl)propane-1,3-dione, $C_{22}H_{18}O_3$,
β-diketone interactions. Part 4. The structures and properties of 1,3-diphenyl-2-methylpropane-1,3-dione, $C_{16}H_{14}O_2$, and 1,3-diphenyl-2-(4-methoxyphenyl) propane-1,3-dione, $C_{22}H_{18}O_3$ 181
1,3-Diphenyl-2-methylpropane-1,3-dione, $C_{16}H_{14}O_2$,
β-diketone interactions. Part 4. The structures and properties of 1,3-diphenyl-2-methylpropane-1,3-dione, $C_{16}H_{14}O_2$, and 1,3-diphenyl-2-(4-methoxyphenyl) propane-1,3-dione, $C_{22}H_{18}O_3$ 181

Fluorobutenes,
molecular mechanics calculations for conformational energies and torsional force constants in fluoropropenes and butenes 283
Fluoromethanes,
dipole moment derivatives and infrared intensities in fluoromethanes 297
Fluoropropenes,
molecular mechanics calculations for conformational energies and torsional force constants in fluoropropenes and butenes 283

Germyl halides,
intramolecular coupling of vibrational modes and the assignments of the partially-deuterated methyl, silyl and germyl halides 245

HCl,
dipole moment functions of van der Waals complexes of HF and HCl with rare gas atoms 321
HF,
dipole moment functions of van der Waals complexes of HF and HCl with rare gas atoms 321

{[HN—$(CH_2)_2$—NH]$N_3P_3Cl_3$}$_2$[HN—$(CH_2)_n$—NH] cyclophosphazenic species,
202 MHz ^{31}P NMR performances, Part II. The challenge of the {[HN—$(CH_2)_2$—NH]$N_3P_3Cl_3$}$_2$[HN—$(CH_2)_n$—NH] cyclophosphazenic species 175
Hydrogen bonding,
hydrogen bonding. Part 24. Dichotomous hydration behavior of quaternary ammonium halides 205
Hydrogen bonds,
influence of phenol acidity and solvent polarity with phenol—retinal Schiff base hydrogen bonds — thermodynamic parameters of bond formation and proton transfer 87

$I^- \cdot SO_2$,
the pre-resonance Raman effect of the species $I^- \cdot SO_2$ and $SCN^- \cdot SO_2$ 15

Ketene,
the ground state average structure of ketene 311

Matrix isolated molecules,
site selective thermal stereoisomerization of matrix isolated molecules: simulation by molecular mechanics 265
Methyl halides,
intramolecular coupling of vibrational modes and the assignments of the partially-deuterated methyl, silyl and germyl halides 245
Morpholinium pentachlorophenolate monohydrate,
the structure and spectroscopic behavior of morpholinium pentachlorophenolate monohydrate 165

Norbornadiene,
a re-interpretation of the uv-photoelectron spectra of Dewar benzene, norbornadiene and barrelene by ab initio configuration interaction calculations 333

2,2,5,5,6,6,9,9-Octamethyl-3-7-decadiyne,
the conformations and vibrational spectra of 2,2,5,5,6,6,9,9-octamethyl-3-7-decadiyne 63

Perfluoro-norbornadiene,
the molecular structure of perfluoro-norbornadiene: a gas phase electron diffraction study 105
Permethrinic acid esters,
effect of molecular structure on stereoselectivity during the hydrolysis of diastereoisomeric permethrinic acid esters 111
3-Phenethyl-3-azabicyclo[3.2.1]octan-8-β-ol,
structural and conformational study of 3-phenethyl-3-azabicyclo[3.2.1]octan-8-β-ol 151
2-Phenylimino-3,1-perhydrobenzoxazines,
on the tautomerism and conformational characteristics of 2-phenylimino-3,1-perhydrobenzoxazines and analogous benzothiazines: an X-ray study 125

Quaternary ammonium halides,
hydrogen bonding. Part 24. Dichotomous hydration behavior of quaternary ammonium halides 205

$SCN^- \cdot SO_2$,
the pre-resonance Raman effect of the species $I^- \cdot SO_2$ and $SCN^- \cdot SO_2$ 15
Silyl halides,
intramolecular coupling of vibrational modes and the assignments of the partially-deuterated methyl, silyl and germyl halides 245

2,3,4,5-Tetrasubstituted pyrrolidines,
NMR spectra and stereochemistry of some 2,3,4,5-tetrasubstituted pyrrolidines 231
Trans-[$PtX_2(C_2H_4)$(Him)],
NMR exchange studies on the complexes *trans*-[$PtX_2(C_2H_4)$(Him)] (X = Cl, Br; Him = imidazole) 237
Trichloroacrylic acid, Cl_2O=CClCOOH,
phase transition in trichloroacrylic acid, Cl_2O=CClCOOH. An X-ray diffraction ^{35}Cl-nuclear quadrupole resonance and pyroelectricity study 139
1,3,5-Trideuterobenzene, $C_6^1H_3^2H_3$,
the pure rotational Raman spectrum of 1,3,5-trideuterobenzene, $C_6^1H_3^2H_3$ 23

CONTENTS

Vibrational study of structures and phase transitions in caesium hydrogen selenate ($CsHSeO_4$)
Ph. Colomban (Palaiseau, France), M. Pham-Thi and A. Novak (Thiais, France) 1
The pre-resonance Raman effect of the species $I^- \cdot SO_2$ and $SCN^- \cdot SO_2$
P. S. Santos, D. L. A. Faria and J. G. N. Santos (São Paulo, Brazil). 15
The pure rotational Raman spectrum of 1,3,5-trideuterobenzene, $C_6^1H_3^2H_3$
H. G. M. Edwards (Bradford, Gt. Britain) 23
Vibrational spectra of diacetylene and its deuterated species
N. L. Owen, C. H. Smith and G. A. Williams (Gwynedd, Gt. Britain). 33
Conformational enthalpy and volume changes in bromocyclohexane determined by Raman spectroscopy
D. J. Gardiner and N. A. Walker (Newcastle upon Tyne, Gt. Britain). 55
The conformations and vibrational spectra of 2,2,5,5,6,6,9,9-octamethyl-3-7-decadiyne
A. Horn, P. Klaeboe, C. J. Nielsen (Oslo, Norway) and W. Aehle (Braunschweig, F.R.G.). 63
Surface enhanced Raman study of benzidine on a silver electrode: an interpretation for different adsorption configurations at various applied voltages
L. Guohai and W. Guozhen (Beijing, China) 75
Influence of phenol acidity and solvent polarity with phenol—retinal Schiff base hydrogen bonds — thermodynamic parameters of bond formation and proton transfer
H. Schmideder, O. Kasende, H. Merz, P. P. Rastogi and G. Zundel (Munich, F.R.G.) 87
The molecular structure and conformation of 1,1′-dimethyl-bicyclopropyl
A. de Meijere (Hamburg, F.R.G.) and M. Traetteberg (Dragvoll, Norway) 97
The molecular structure of perfluoro-norbornadiene: a gas phase electron diffraction study
B. Beagley, R. K. Knowles and R. G. Pritchard (Manchester, Gt. Britain) 105
Effect of molecular structure on stereoselectivity during the hydrolysis of diastereoisomeric permethrinic acid esters
K. Simon, I. Boros, G. Balogh, G. Hidasi, E. Fogassy, F. Faigl and M. Ács (Budapest, Hungary) 111
On the tautomerism and conformational characteristics of 2-phenylimino-3,1-perhydrobenzoxazines and analogous benzothiazines: an X-ray study
A. Kálmán, Gy. Argay (Budapest, Hungary), F. Fülöp and G. Bernáth (Szeged, Hungary) 125
Phase transition in trichloroacrylic acid, $Cl_2C{=}CClCOOH$: an X-ray diffraction, ^{35}Cl-nuclear quadrupole resonance and pyroelectricity study
S. Fleck, R. Göckel and A. Weiss (Darmstadt, F.R.G.) 139
Structural and conformational study of 3-phenethyl-3-azabicyclo[3.2.1]octan-8-β-ol
M. S. Arias, E. Galvez, I. Ardid, J. Bellanato, J. V. Garcia-Ramos, F. Florencio and S. Garcia-Blanco (Madrid, Spain) 151
The structure and spectroscopic behavior of morpholinium pentachlorophenolate monohydrate
I. Majerz, Z. Malarski and T. Lis (Wrocław, Poland) 165
202 MHz ^{31}P NMR performances. Part II. The challenge of the $\{[HN{-}(CH_2)_2{-}NH]N_3P_3Cl_3\}_2[HN{-}(CH_2)_n{-}NH]$ cyclophosphazenic species
B. Perly, P. Berthault (Gif-sur-Yvette, France), L. Vidaud, J.-P. Bonnet and J.-F. Labarre (Toulouse, France). 175
β-Diketone interactions. Part 4. The structures and properties of 1,3-diphenyl-2-methylpropane-1,3-dione, $C_{16}H_{14}O_2$, and 1,3-diphenyl-2-(4-methoxyphenyl)propane-1,3-dione, $C_{22}H_{18}O_3$
J. Emsley, N. J. Freeman, M. B. Hursthouse and P. A. Bates (London, Gt. Britain) 181
β-Diketone interactions. Part 5. Solvent effects on the keto ⇌ enol equilibrium
J. Emsley and N. J. Freeman (London, Gt. Britain) 193
Hydrogen bonding. Part 24. Dichotomous hydration behavior of quaternary ammonium halides
K. M. Harmon, G. F. Avci and A. C. Thiel (Rochester, MI, U.S.A.). 205
Single crystal Zeeman effect studies on ^{35}Cl NQR lines of 2,6-dichlorophenol
N. V. L. N. Prasad, P. Venkatacharyulu and D. Premaswarup (Nagarjunanagar, India). 219
NMR spectra and stereochemistry of some 2,3,4,5-tetrasubstituted pyrrolidines
B. Mikhova, S. L. Spassov, K. Popandova, V. Dryanska, C. Ivanov (Sofia, Bulgaria), H. Duddeck and M. Kaiser (Bochum, F.R.G.). 231

(Continued overleaf)

(*Contents continued*)

NMR exchange studies on the complexes *trans*-[$PtX_2(C_2H_4)$(Him)] (X = Cl, Br; Him = imidazole)
G. A. Foulds, P. S. Hall and D. A. Thornton (Rondebosch, South Africa) 237
Intramolecular coupling of vibrational modes and the assignments of the partially-deuterated methyl, silyl and germyl halides
J. S. Weaving and T. A. Ford (Wits, South Africa) 245
Site selective thermal stereoisomerization of matrix isolated molecules: simulation by molecular mechanics
S. Charbonnier, R. Viani (Abidjan, Ivory Coast), J. Pourcin and H. Bodot (Marseille, France) 265
Molecular mechanics calculations for conformational energies and torsional force constants in fluoropropenes and butenes
P. J. Stavnebrekk and R. Stølevik (Dragvoll, Norway) 283
Dipole moment derivatives and infrared intensities in fluoromethanes
K. Kim and C. W. Park (Seoul, Korea) 297
The ground state average structure of ketene
J. L. Duncan and B. Munro (Old Aberdeen, Scotland) 311
Dipole moment functions of van der Waals complexes of HF and HCl with rare gas atoms
M. O. Bulanin, V. P. Bulychev and K. G. Tokhadze (Leningrad, U.S.S.R.). 321
A re-interpretation of the uv-photoelectron spectra of Dewar benzene, norbornadiene and barrelene by ab initio configuration interaction calculations
M. H. Palmer (Edinburgh, Gt. Britain) 333

Book Reviews 347

Publications Received 352